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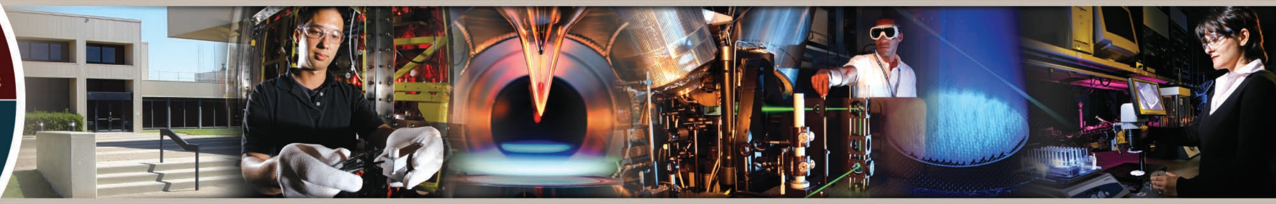

May/June 2008 • VOL. 30, NO. 3

Analysis of barriers for mitigation of unintended releases of hydrogen

The development and commercial use of hydrogen will require safety guidelines for building vehicle fueling stations, storage facilities, and other infrastructure components. If the development of these safety guidelines is to be made on a scientific basis, then validated engineering models of unintended hydrogen releases are needed for scenario and risk analysis.

Hydrogen jet flames resulting from the ignition of unintended releases can be extensive in length and pose significant radiation and impingement hazards (Schefer et. al., 2006). Depending on the leak diameter and source pressure, the resulting consequence distances can be unacceptably large. One mitigation strategy for reducing the exposure to flames that can occur with unintended releases is to incorporate barriers around hydrogen storage equipment. The reasoning is that walls will reduce the extent of unacceptable consequences due to jet releases resulting from accidents involving high-pressure equipment. While reducing the jet extent, the walls may introduce other hazards if not properly configured. A Sandia team consisting of Robert Schefer, Bill Houf and Greg Evans is working to develop the technical expertise needed to guide the configuration and placement of these walls to minimize overall hazards and to provide quantitative information on barrier hazard distance reduction for use in safety guideline risk analysis. The experimental effort is complemented by a parallel numerical modeling effort that considers the interaction of jet flames and unignited jets with barriers and the ignition overpressure. Results from the experiments are used to validate the Navier-Stokes simulations of barrier wall impingement and overpressure and provide a measure of confidence in the extension of the simulation capabilities to more complex barrier wall designs and release conditions.

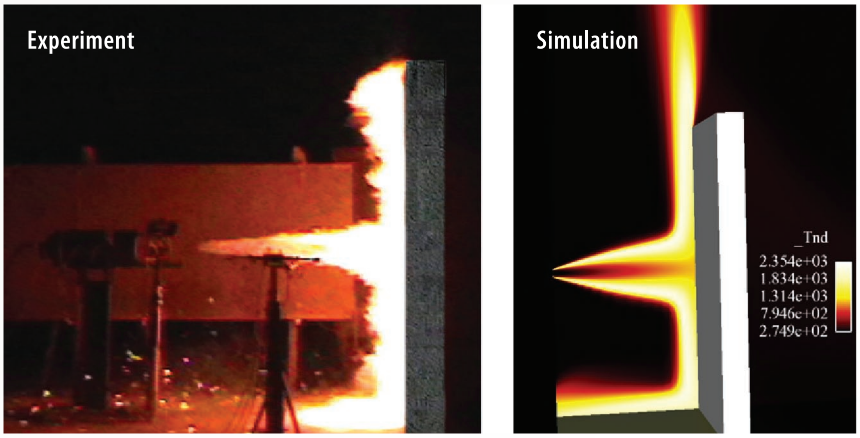

Figure 1. Standard video frames from barrier wall tests at SRI Corral Hollow Test site. Top left: Jet centered on single-wall vertical barrier.

The tests were carried out at the SRI International Corral Hollow test site in Tracy, CA. The barrier wall configurations studied included (1) a single vertical wall with a hydrogen jet centered on the wall; (2) a single wall with the jet located at the top of the wall; (3) a wall inclined at 60 degrees to the horizontal with the jet centered on the wall; and (4) a three-wall barrier

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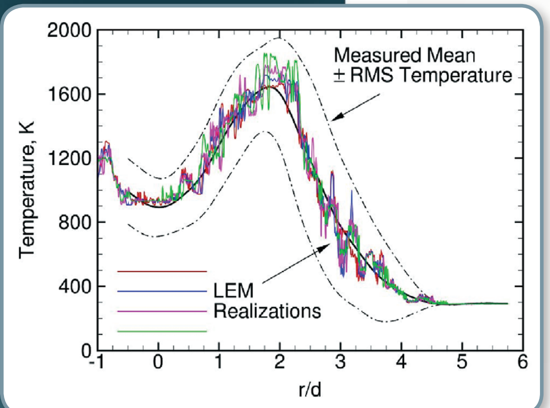
A tabulated closure for nonpremixed combustion using the linear eddy model

Numerical simulations of turbulent combustion processes remain a challenge because of the wide range of length and time scales that must be taken into account. The Large Eddy Simulation (LES) technique accounts for this wide range by resolving the large energetic scales directly and modeling the small "subgrid" scales. This technique allows investigators to simulate realistic operating conditions and device-scale geometries in a computationally feasible manner. The accuracy of LES inherently depends on the subgrid models employed, and thus development of these models is currently an active research topic for many applications. CRF researchers Vaidya Sankaran, Tom Drozda and

Figure 1. Experimental mean plus/minus RMS temperature at x/d = 20 in the DLR flame with four superimposed realizations from LEM.



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Newsletter

Analysis of barriers (continued)

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with a 135 degree angle between adjacent walls. Data were also obtained in a free jet with no wall present to serve as a base case. These tests provide a direct evaluation of barrier effectiveness for mitigation of flame hazards associated with accidental hydrogen leaks as well as providing data for model validation.

Standard visible video recordings were used to characterize the flame size and length and the effectiveness of the barrier at deflecting the hot flame gases. A single video frame taken of the vertical 2.4 m x 2.4 m cinderblock wall, with a centered horizontal hydrogen jet flame, is shown in the left image of Figure 1. The video image shows a 90 degree upward deflection of the flame, with no apparent flame stabilized behind the wall. The part of the flame that is deflected downward by the wall is seen to turn back toward the jet source as it impacts the ground.

A model simulation of the same configuration in shown in the

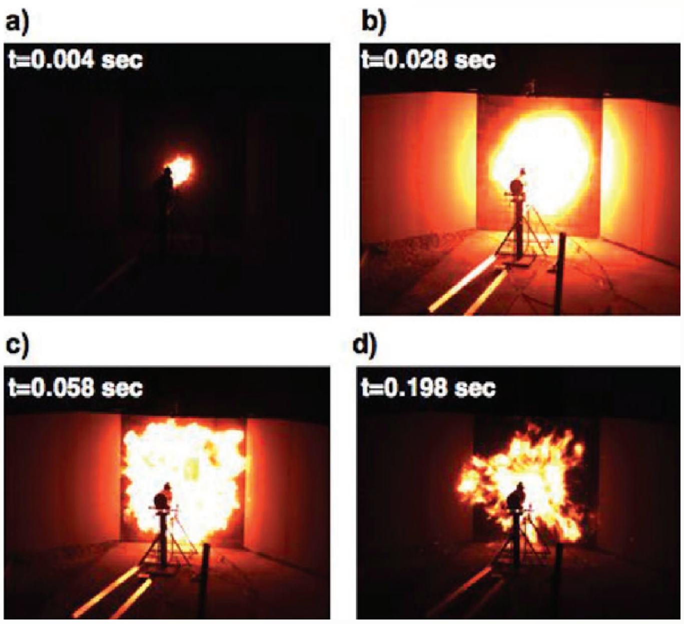

Figure 2. *High speed (500 fps) video frames from three-sided wall test at 4 msec, 28 msec, 58 msec and 94 msec from ignition spark firing.*

right image of Figure 1. The calculations were performed with the Sandia developed code, FUEGO, designed to simulate turbulent, reacting flow and heat transfer (Moen et al., 2002) on massively parallel computers, with a primary focus on heat transfer to objects in pool fires. The code has been adapted for compressible flow and hydrogen combustion. The simulation does an excellent job of predicting the flame deflection due to the presence of the wall in all configurations tested.

The high-speed movies reveal some of the detailed structure associated with the transient flame/wall interactions immediately after flame ignition. Figure 2 shows four frames from the high-speed video movie for the three-wall test. The camera was located behind the hydrogen jet exit and looking toward the wall. The movie was taken at a rate of 500 frames per second. The frame in Figure 2(a) corresponds to a time of 4 msec after the ignition spark occurs. The flame originating at the location of the spark is in the initial stages of propagating outward through the mixture of surrounding hydrogen and air. At t=28 msec the flame "ball" has increased significantly in size and has a diameter nearly equal to the 2.4 m width of the central cinderblock wall. This frame corresponds to the time at which the flame ball diameter is maximum. At t=58 msec irregular edges begin to form around the outer circumference of the flame and the central part of the flame ball begins to exhibit small variations in intensity. Finally, at t=198 msec the edges of the flame are considerably more irregular and convoluted. A similar, irregular structure is also noted throughout the central region of the flame and is characteristic of flow turbulence.

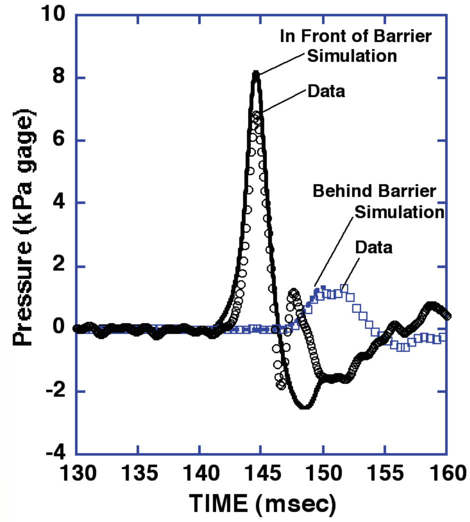

Figure 3. *Comparison of simulation of overpressure from ignition of impinging hydrogen jet on the center of a 1-wall vertical barrier with pressure transducer measurements.*

One potential hazard associated with the use of barrier walls is the overpressure produced from the ignition of an impinging jet release into a barrier and how that pressure is attenuated by the barrier. Simulations of jet releases into the barrier configurations were performed using the FLACS (2003) Navier-Stokes code. Figure 3 shows a comparison of the predicted and simulated overpressure pulse at a location on the front side of the wall (jet side) and at a location on the back side of the wall for the single vertical-wall barrier. The results show that the predicted peak overpressures on both the front and back sides of the wall are in good agreement with the measurements.

Further comparisons of the various wall configurations show that the presence of a wall generally increases the overpressure in front of the wall, but can also reduce pressures behind the wall by up to an order of magnitude.

References

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Moen, C.D., Evans, G.H., Domino, S.P. and Burns, S.P., "A Multi-Mechanics Approach to Computational Heat Transfer," Proceedings 2002 ASME Int. Mech. Eng. Congress and Exhibition, New Orleans, IMECE2002-33098, Nov. 17-22, 2002.

FLACS Version 8 Users Guide, GEXCON, Bergen, Norway, 2003.

Combustion Research Facility Visitor Program

These Sandian researchers will be leaving the CRF at the completion of their tenure.

Alan Elder
Post Doc
Cambridge University, UK
Project: Fluorescence Lifetime Imaging
Mentor: Jonathan Frank

Andrea Gruber
Visiting Researcher
SINTEF Energy Research, Norway
Project: Direct Numerical Simulation of Turbulent Reactive Channel Flow
Host: Jackie Chen

Wontae Hwang
Post Doc
Stanford University
Mentor: John Dec

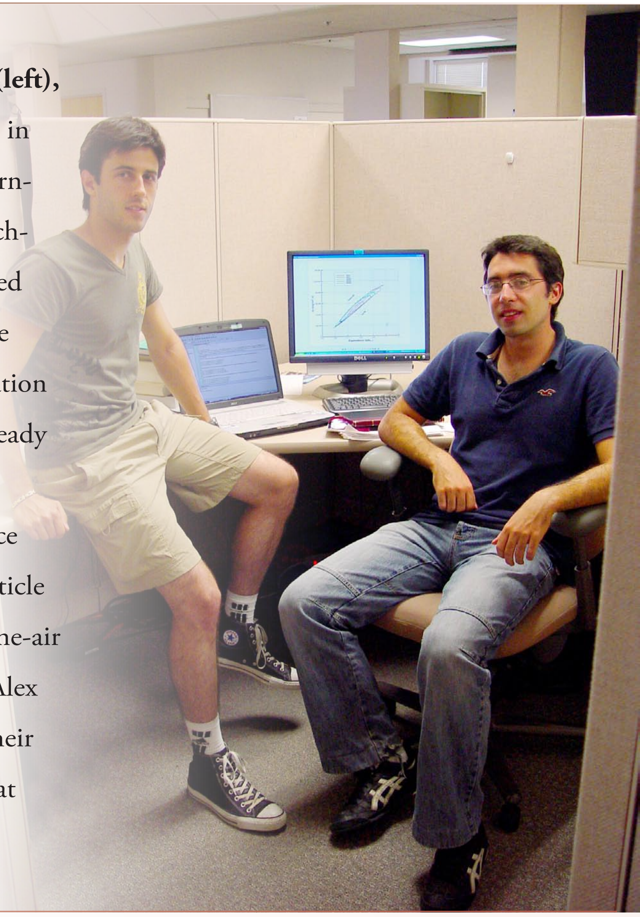
Jane Hwang
Summer Intern
United States Air Force Academy
Host: Carl Hayden

Paul Jansen
Visiting Student
Vrije University, Netherlands
Project: Molecular Bean Scattering of Molecules
Host: Dave Chandler

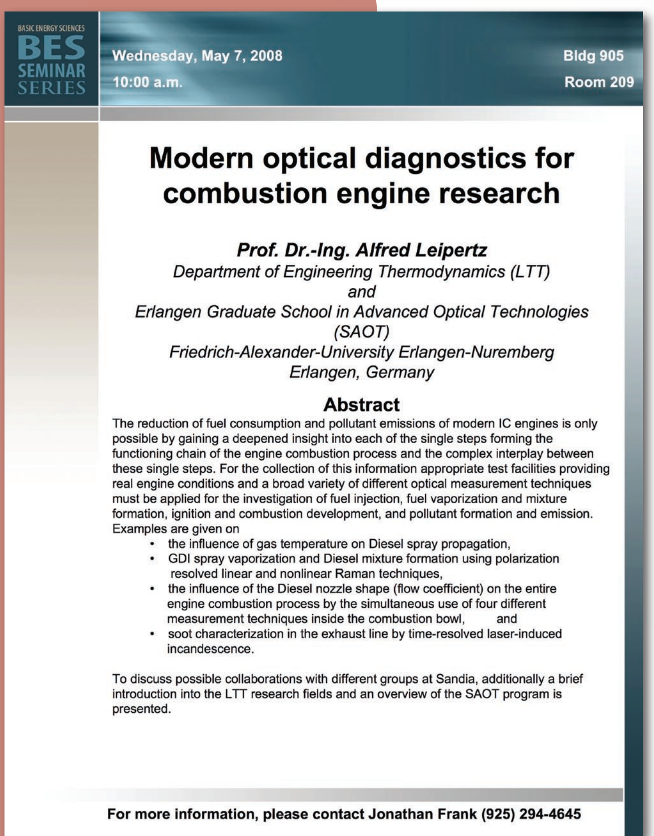
Wim Roeterdink
Visiting Researcher
Vrije University, Netherlands
Project: Ion Imaging
Host: Carl Hayden and Dave Chandler

Sigurd Sannan
Visiting Researcher
SINTEF Energy Research, Norway
Project: Computational Model of Turbulent Combustion
Host: Jackie Chen

CRF interns



Victor Granet (right) and Alexandre Eyssartier (left), Masters students from the University of Enseeight in France, have recently completed a six months internship at the CRF mentored by Jackie Chen, Ed Richardson and Chun Sang Yoo. They have investigated the effects of equivalence ratio stratification on the flame structure, NO formation, and propagation of strained lean methane-air flames in unsteady strained counterflow simulations. In addition, they are investigating the performance of micro-mixing models from Lagrangian particle tracking in DNS of a lifted autoigniting ethylene-air jet flame in a heated coflow. Both Victor and Alex will return to France where they will pursue their Ph.D. studies with Professor Thierry Poinsot at CERFACS in Toulouse.



BASIC ENERGY SCIENCES
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Wednesday, May 7, 2008
10:00 a.m.

Bldg 905
Room 209

Modern optical diagnostics for combustion engine research

Prof. Dr.-Ing. Alfred Leipertz
Department of Engineering Thermodynamics (LTT)
and
Erlangen Graduate School in Advanced Optical Technologies (SAOT)
Friedrich-Alexander-University Erlangen-Nuremberg
Erlangen, Germany

Abstract

The reduction of fuel consumption and pollutant emissions of modern IC engines is only possible by gaining a deepened insight into each of the single steps forming the functioning chain of the engine combustion process and the complex interplay between these single steps. For the collection of this information appropriate test facilities providing real engine conditions and a broad variety of different optical measurement techniques must be applied for the investigation of fuel injection, fuel vaporization and mixture formation, ignition and combustion development, and pollutant formation and emission. Examples are given on

- the influence of gas temperature on Diesel spray propagation,
- GDI spray vaporization and Diesel mixture formation using polarization resolved linear and nonlinear Raman techniques,
- the influence of the Diesel nozzle shape (flow coefficient) on the entire engine combustion process by the simultaneous use of four different measurement techniques inside the combustion bowl, and
- soot characterization in the exhaust line by time-resolved laser-induced incandescence.

To discuss possible collaborations with different groups at Sandia, additionally a brief introduction into the LTT research fields and an overview of the SAOT program is presented.

For more information, please contact Jonathan Frank (925) 294-4645

BES lecturer Dr. Alfred Leipertz

On May 7th, invited guest speaker Professor Alfred Leipertz, Department of Engineering Thermodynamics (LTT) and Erlangen Graduate School in Advanced Optical Technologies (SAOT), Friedrich-Alexander University Erlangen-Nuremberg, Erlangen, Germany, gave a presentation at the CRF on the topic "Modern optical diagnostics for combustion engine research," as part of the Basic Energy Sciences (BES) annual seminar series. Professor Leipertz provided a brief introduction to LTT research fields and an overview of the SAOT program, and discussed possible collaborations with different groups at Sandia.

A tabulated closure (continued)

(Continued from page 1)

Joe Oefelein are investigating the prospects of developing a novel LES closure for nonpremixed flames, first using experimental line-image data from an actual flame, and using the Linear Eddy Model (LEM) to simulate these data.

The basic assumption for the closure is that small scale features of the scalar field in a turbulent flame are generic in a manner that allows one to approximate them by a scalar field that evolves independently of the underlying large scale flow. In other words, detailed information associated with a scalar field from one nonpremixed flame can be used to predict the small scale structure of another turbulent flame. Given this assumption, one can parameterize the instantaneous structure of a scalar field using a surrogate scalar field with a particular set of properties. Instantaneous realizations of the surrogate field can then be processed directly as a function of key controlling parameters and stored in the form of a library to be used as a subgrid model.

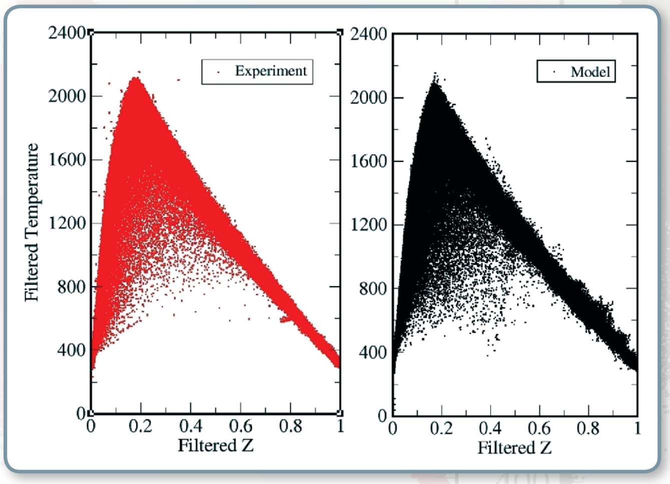

Figure 2. *Scatter plots of filtered temperature obtained from the line-measurement data and from the tabulated closure.*

The effectiveness of the closure postulated above depends on the appropriateness of the chosen parameters. Here, we have postulated that the filtered mixture fraction (Z), filtered scalar dissipation (χ), and subgrid Reynolds number (Re_Δ) are the key parameters. The filtered mixture fraction provides a measure of the relative proportions of the fuel and oxidizer streams (both burned and unburned) by mass. The scalar dissipation provides the rate at which the fuel and oxidizer streams are mixing. Finally, the subgrid Reynolds number indicates the magnitude of the unresolved fluctuations and has been found to provide a good measure of the subgrid scalar dissipation rate. Thus, the combination of filtered scalar dissipation and the subgrid Reynolds number characterize the effect of the total scalar dissipation rate.

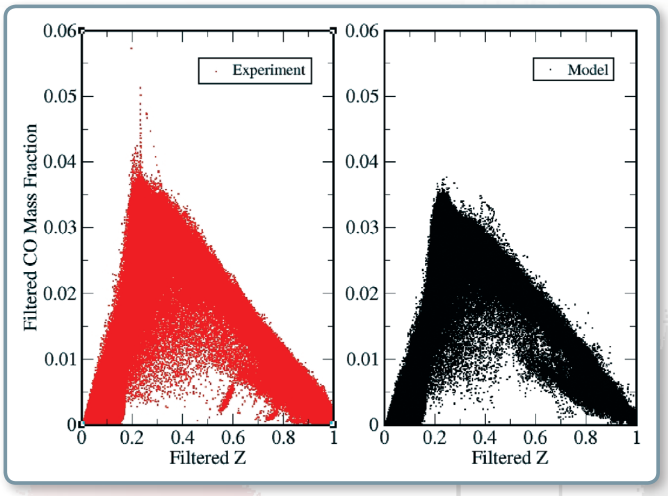

Figure 3. *Scatter plots filtered CO mass fraction obtained from line-measurement data and from the tabulated closure.*

Two steps were taken to validate the parameterization. First, the experimental data obtained using Raman/Rayleigh/CO-LIF technique of a $CH_4/H_2/N_2$ fueled jet flame at $Re_{jet} = 15{,}200$ (i.e., the "DLR-A" flame) were used to construct a table and demonstrate that the parameterization is capable of reproducing the experimental trends. Second, a surrogate scalar field obtained using LEM simulations was used to demonstrate the analogy with the experimental line images. Figure 1 illustrates this analogy graphically. LEM is a 1D scalar mixing model that solves the reaction-diffusion equations with a turbulent advection model to simulate 3D turbulence. Molecular diffusion is treated explicitly, and reaction terms are evaluated in closed form. Turbulent advection is modeled by a stochastic mapping procedure that is characterized by the subgrid Reynolds number. This method yields scalar profiles that are analogous to line-measurement profiles, with statistical and spectral properties similar to the experimentally observed values. The experimental line-image data were used for *a priori* validation of the closure by tabulating it in a manner identical to the analogous signals generated by LEM.

Figures 2 and 3 show scatter plots of the filtered temperature and CO mass fractions obtained from line-measurement data and from the tabulated closure. The scatter plots of the actual experimental data were obtained by filtering the

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A tabulated closure (continued)

(Continued from page 5)

ensemble of scalar profiles. Comparisons between the actual and parameterized data are in good agreement with each other. Increased stretching of the mixture fraction surfaces near the flame region can sometimes cause local extinction if the local scalar dissipation is above a threshold value. This leads to a sudden drop in the local temperature and a sudden increase in the mass fraction of temperature-dependent intermediate species such as CO, as seen in Figure 3. This effect is captured qualitatively by the current tabulated closure.

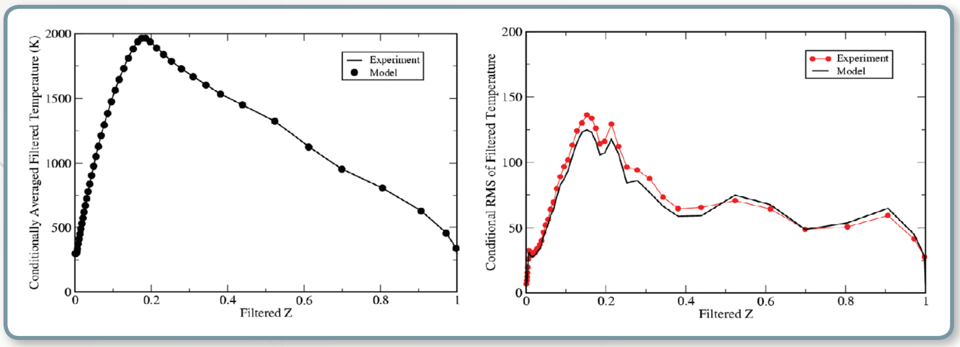

Figure 4. (a) Conditional mean of filtered temperature and (b) conditional RMS of filtered temperature obtained line-measurement data and from the tabulated closure.

Figures 4 (a) and (b) show the conditional mean and conditional RMS of the filtered temperature. Similarly, Figures 5 (a) and (b) show the conditional mean and RMS of CO mass fraction. Once again, the agreement between the tabulated model and the measurements are good and the error in the predicted values of conditional RMS quantities is less than 10%. The agreement between the experiments and LEM are very good, indicating that the LEM simulations have the potential to generate data that are quantitatively similar to the line-measurement data for nonpremixed flames similar to the DLR configuration. A posteriori tests of the tabulated closure using LES are currently underway.

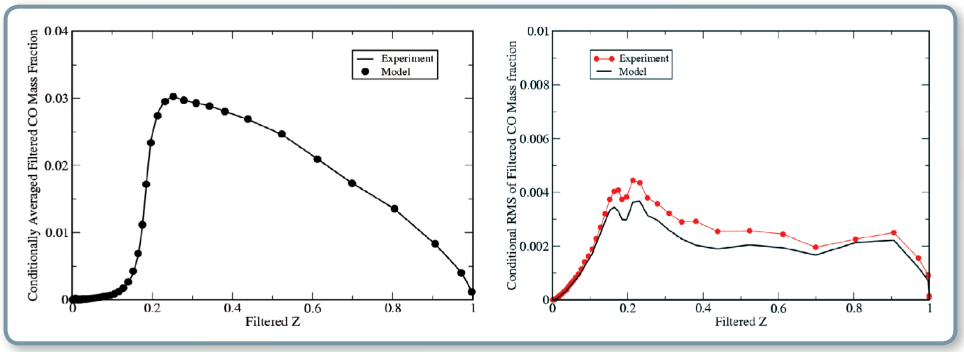

Figure 5. (a) Conditional mean of filtered CO mass fraction and (b) conditional RMS of filtered CO mass fraction obtained line-measurement data and from the tabulated closure

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Subscriptions are free. Subscriptions and address changes to Frank Cebulski, fcebuls@sandia.gov

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